Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supplementary Information: Hydrogen adsorption trends on Al-doped $Ni_2P$ surfaces for optimal catalyst design

Lauri Partanen, Mikko Hakala, and Kari Laasonen*

*Department of Chemistry and Materials Science, Aalto University, P.O. Box 16100, FI-00076 Aalto, Finland*

E-mail: kari.laasonen@aalto.fi

## 1 H-adsorption energies for $Ni_3P_2$ termination of $Ni_2P$

Optimised hydrogen adsorption energies for the first (green triangle) and second (purple square) hydrogens at the 14 investigated hydrogen starting positions (H identifier) on top of the $Ni_3P_2$ terminated $Ni_2P$ slab. The dashed black line indicates the $\Delta G_H$ of the first hydrogen adsorption for the pristine slab, whereas the dashed red line shows the second hydrogen adsorption $\Delta G_H$ value for the pristine slab. As described in the article, the deep yellow band highlights the $\pm 0.1$ eV region around the optimal $\Delta G_H = 0$ value. For example, in Figure S1, the green triangle at H identifier 13 corresponds to the black triangle at Mg (l1d1) in Figure 5 of the main article. Similarly, the purple square at H identifier 1 corresponds to the green square at Mg (l1d1) in the same Figure.

## 1.1 Dopants on a single layer

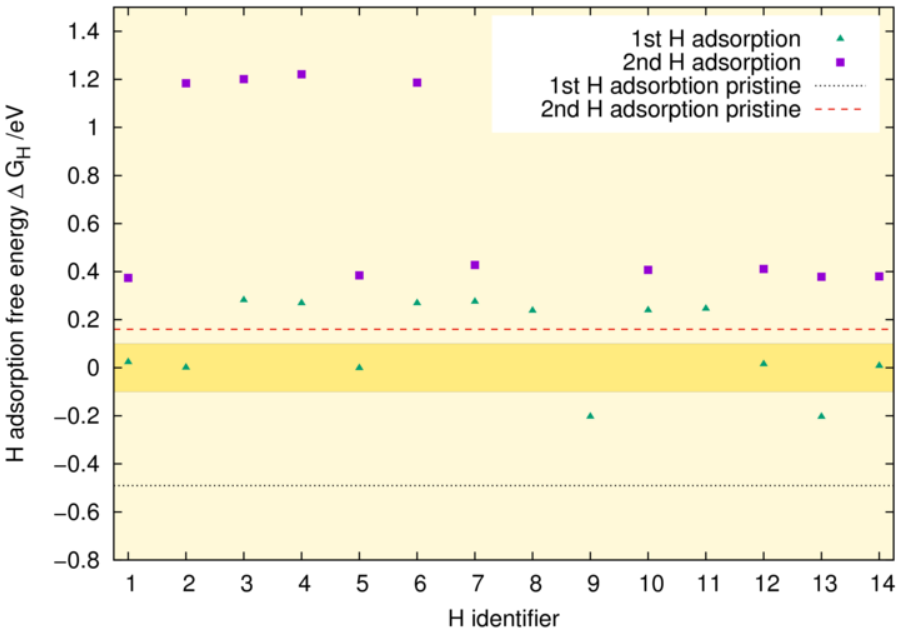


Figure S1: Mg (l1d1)

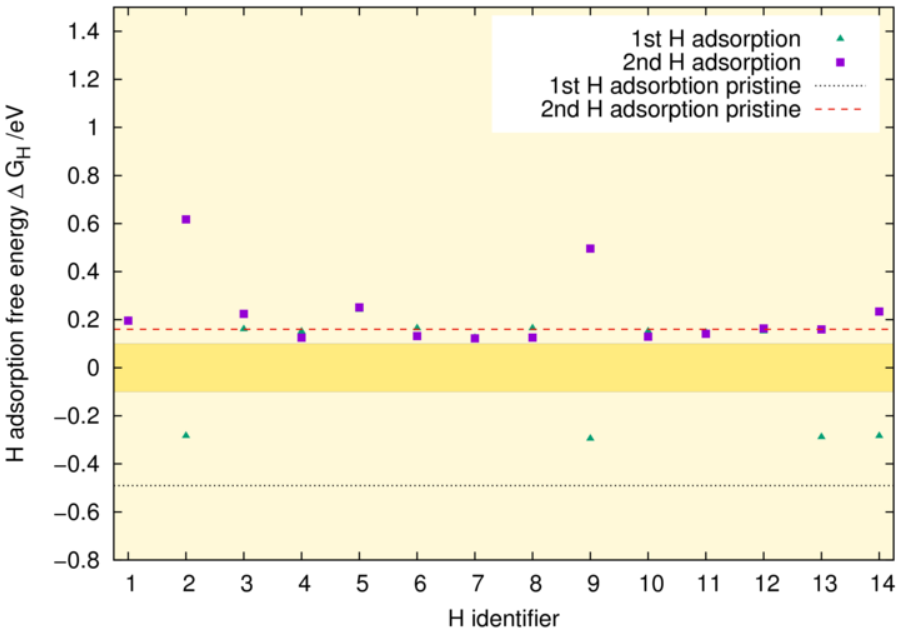


Figure S2: Mg (l2d1)

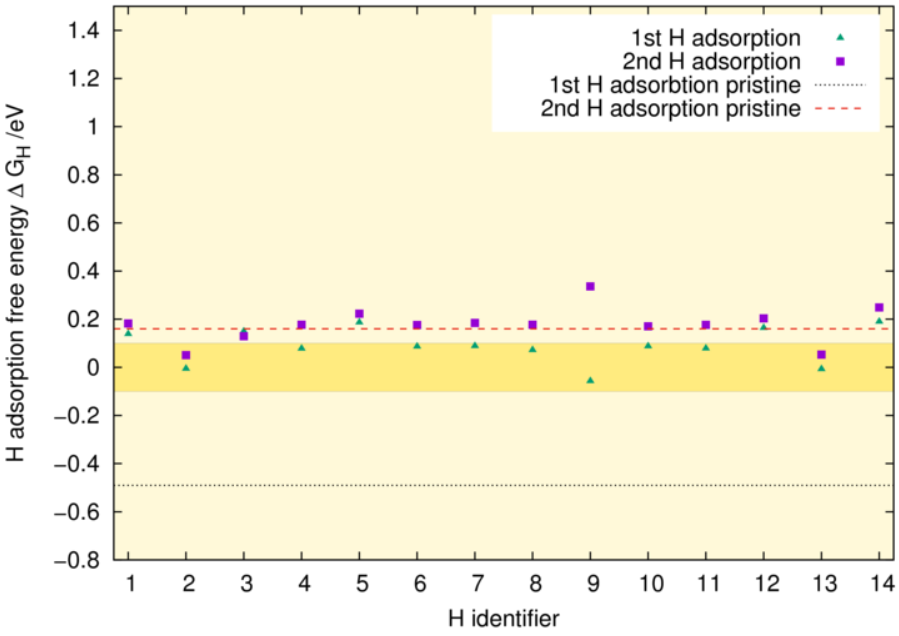


Figure S3: Mg (l2d3)

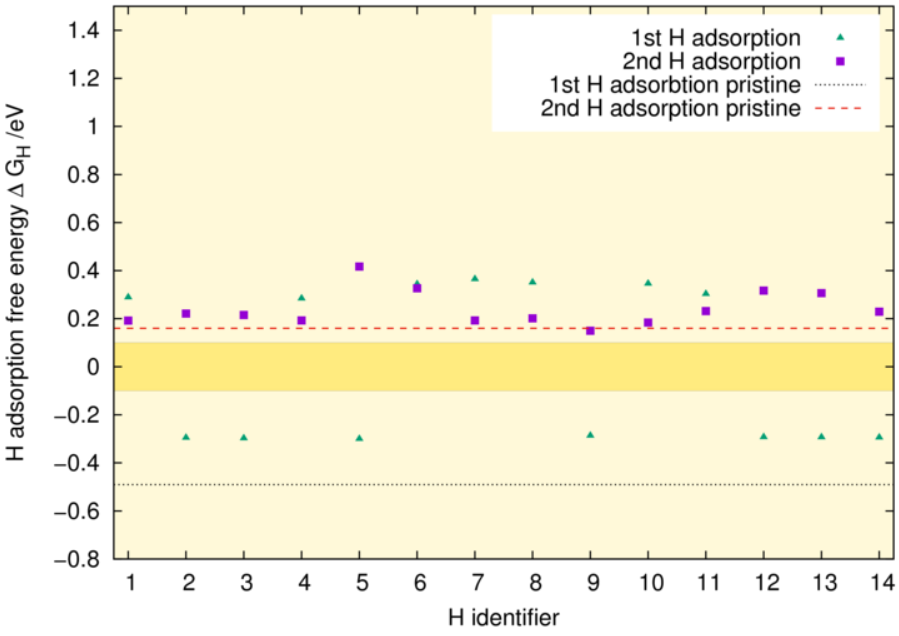


Figure S4: V (l2d1)

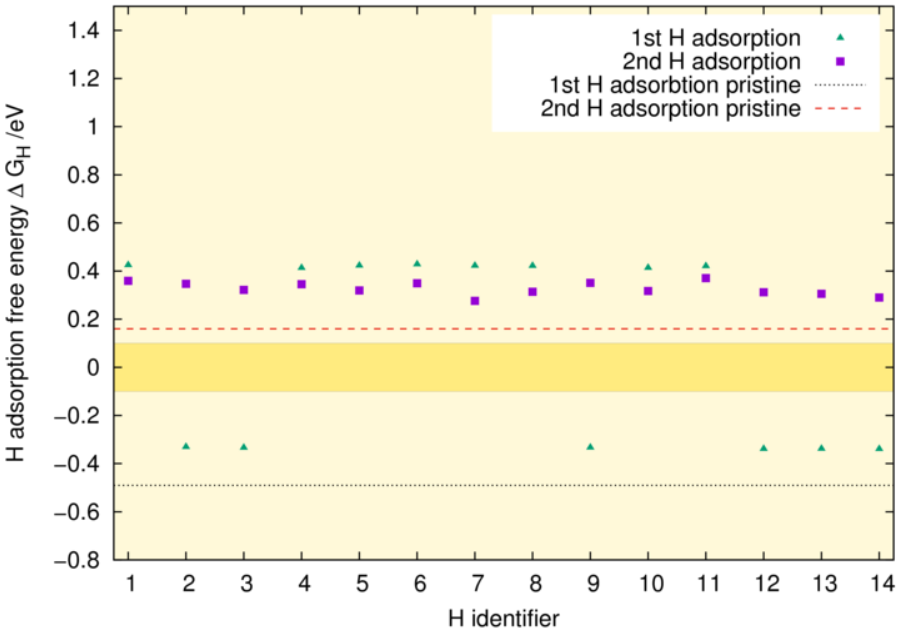


Figure S5: V (l2d3)

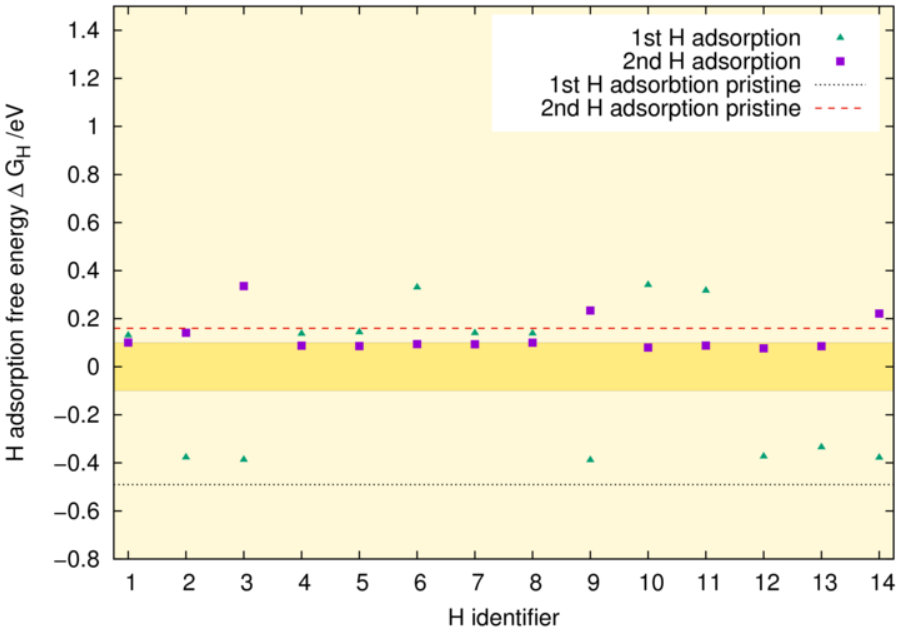


Figure S6: V (l3d1)

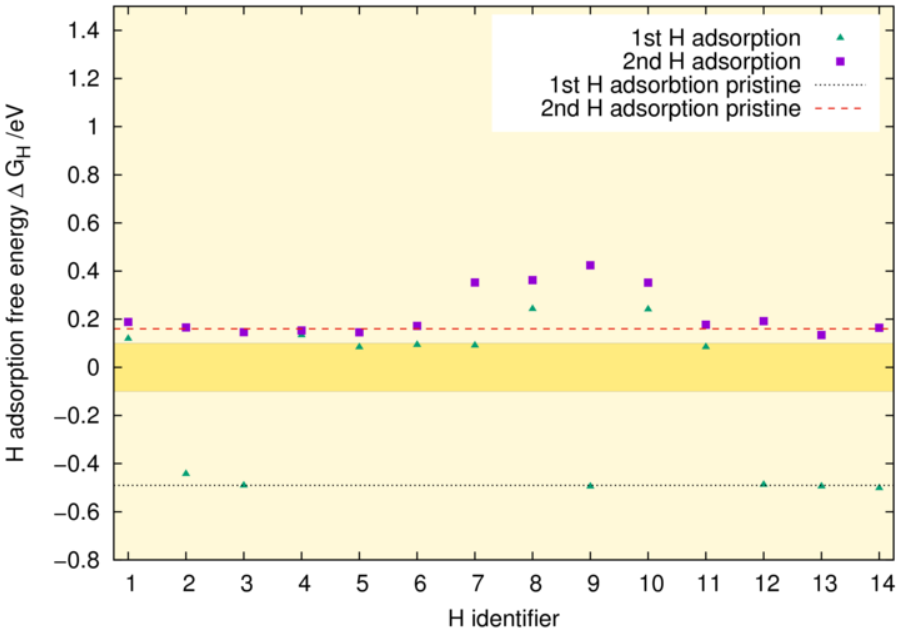


Figure S7: V (l4d1)

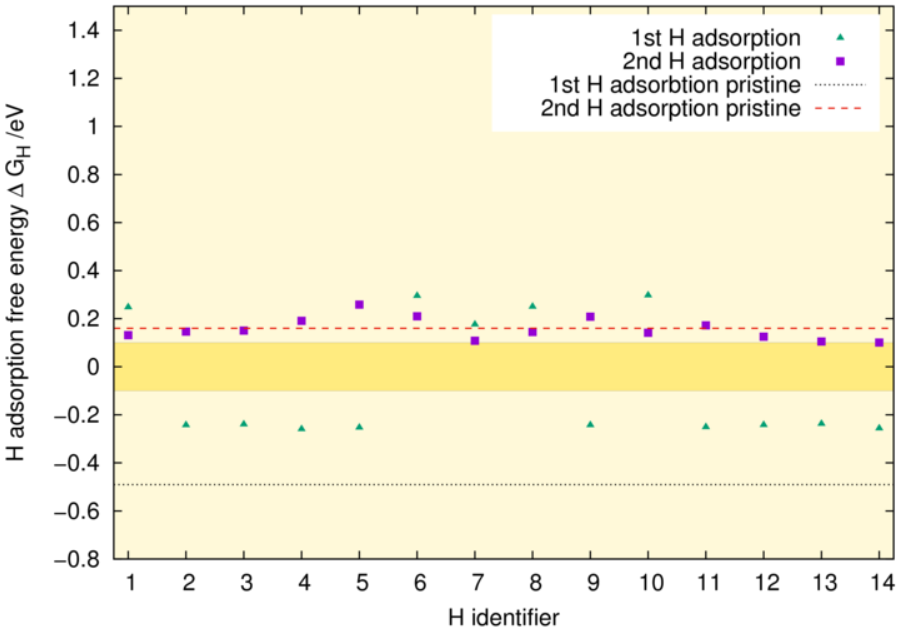


Figure S8: Fe (l2d2)

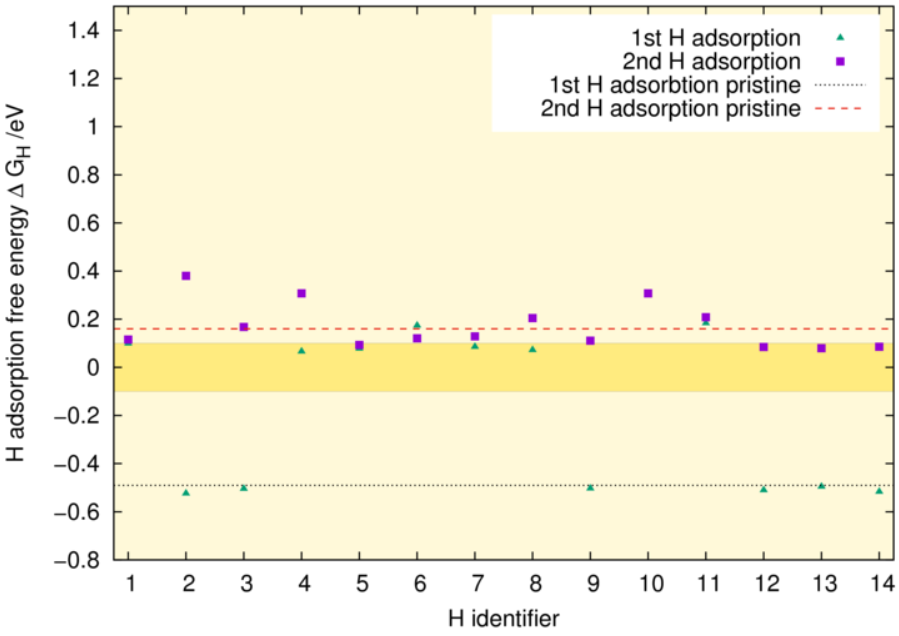


Figure S9: Fe (l3d1)

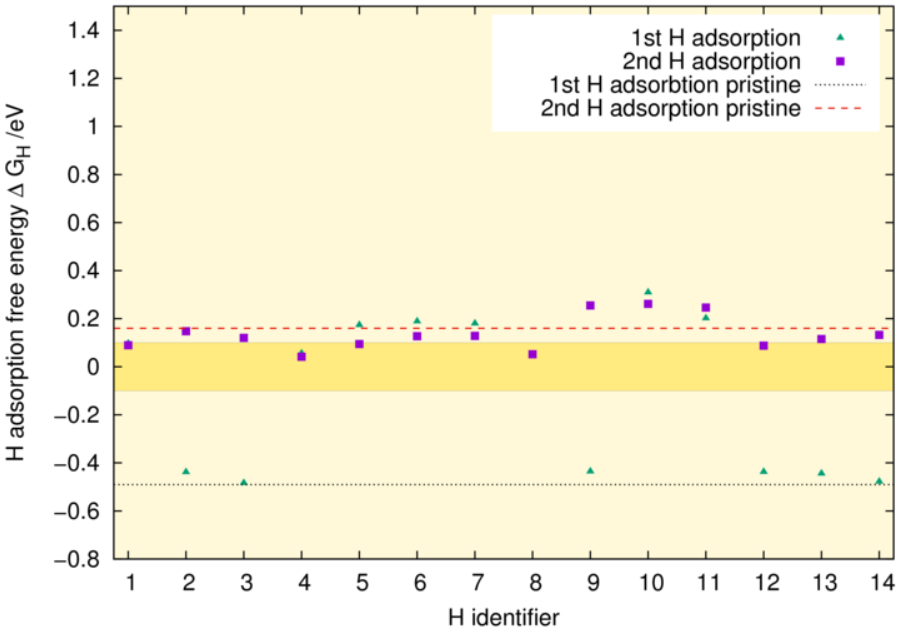


Figure S10: Fe (l3d2)

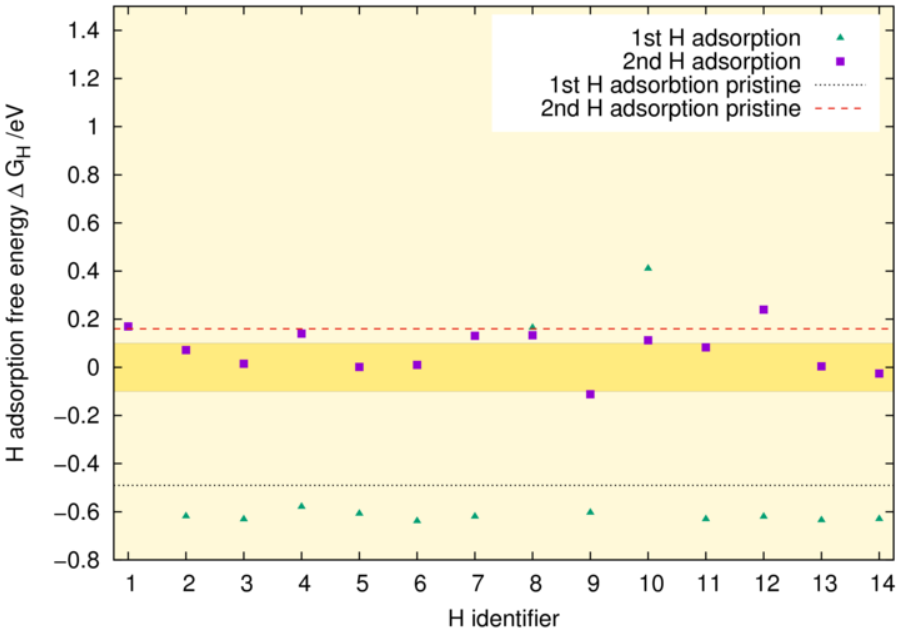


Figure S11: Co (l1d2)

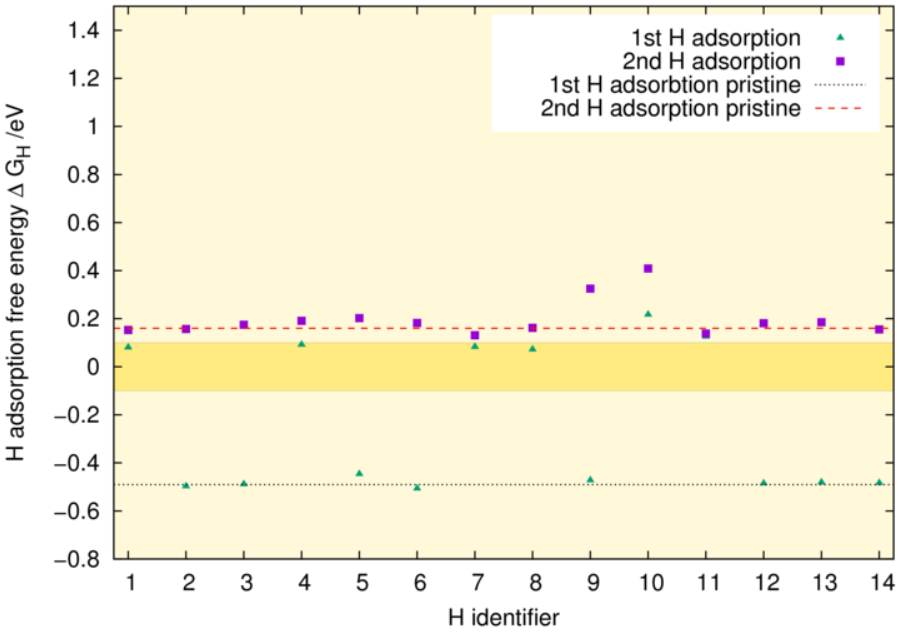


Figure S12: Co (l2d1)

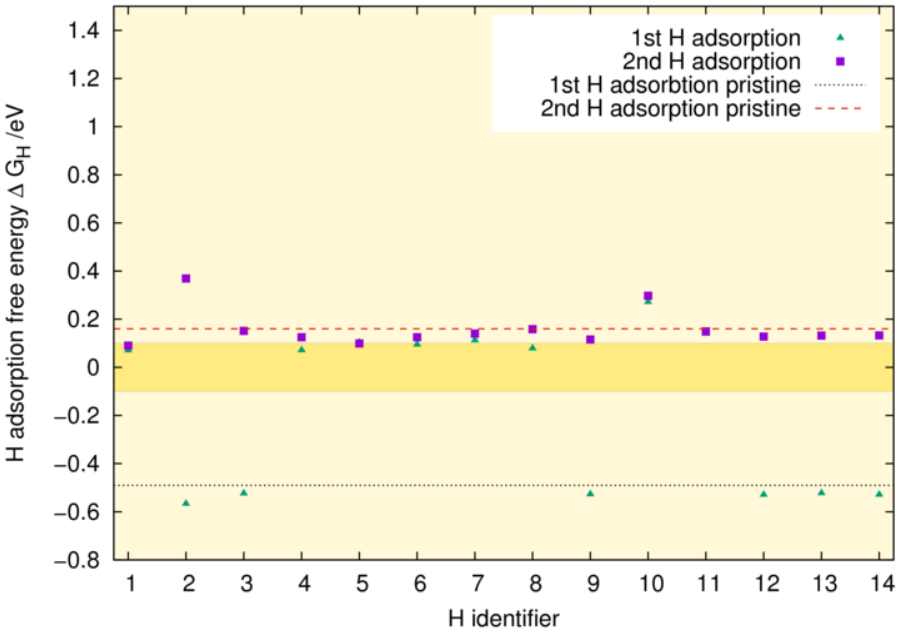


Figure S13: Co (l3d2)

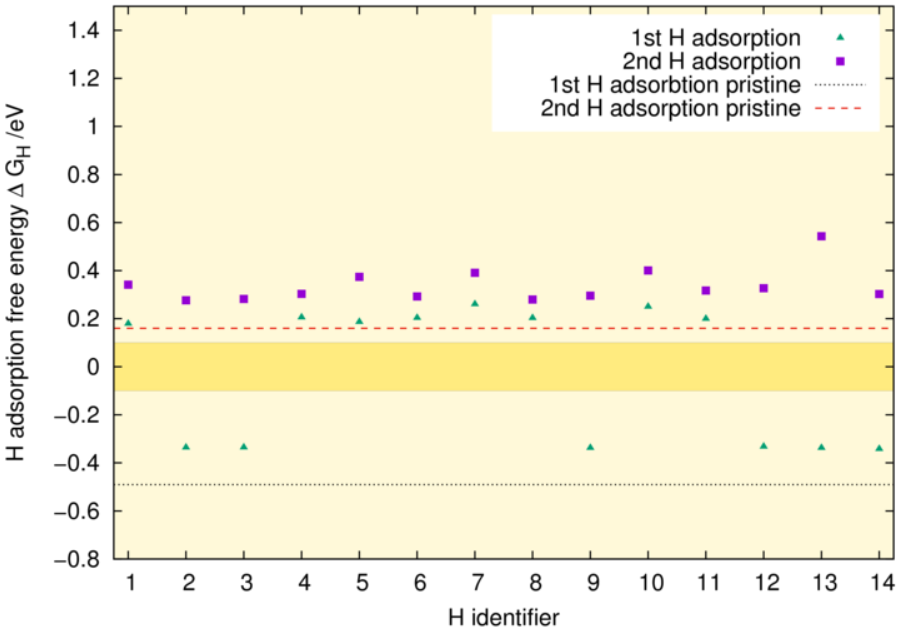


Figure S14: Cu (l1d1)

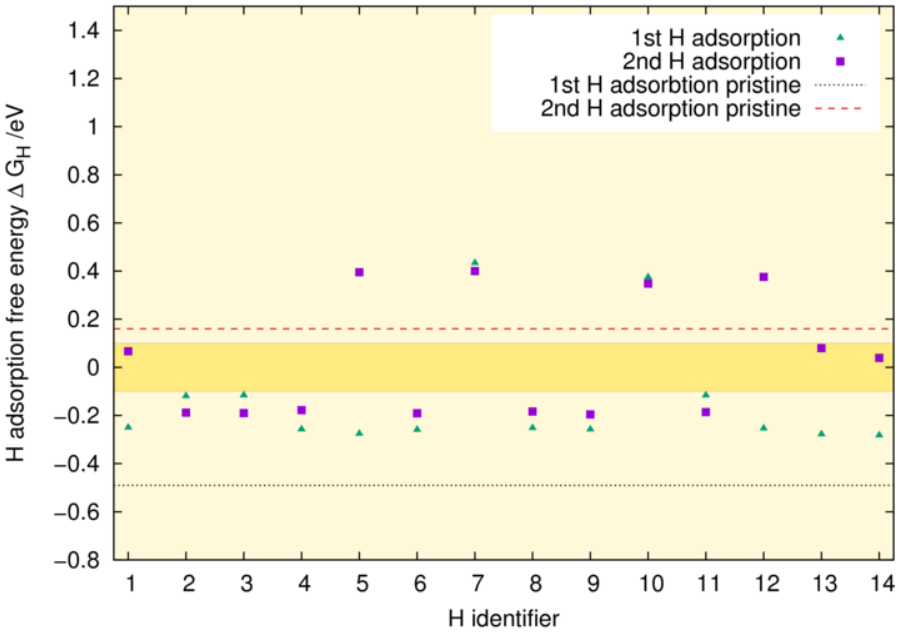


Figure S15: Mo (l1d1)

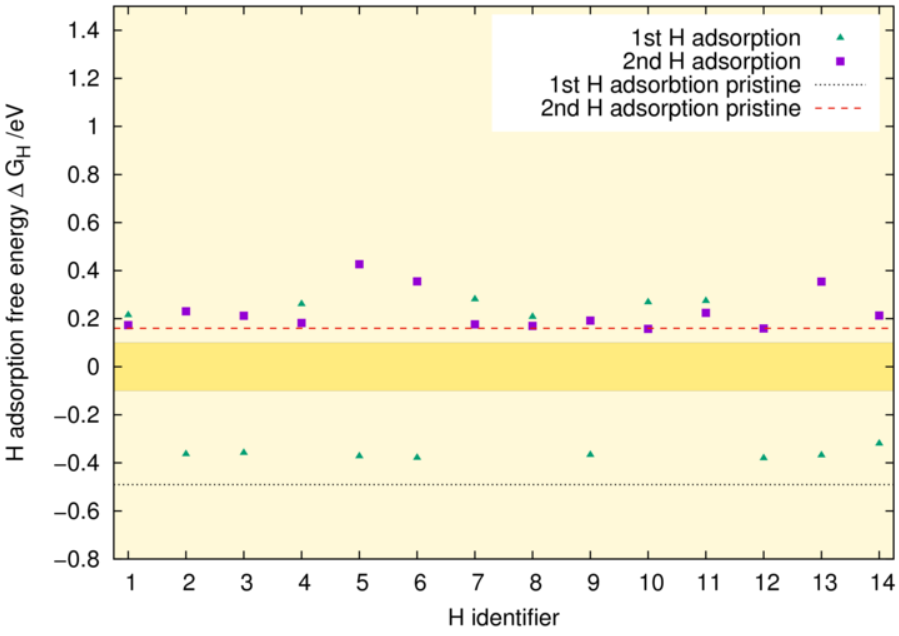


Figure S16: Mo (l2d1)

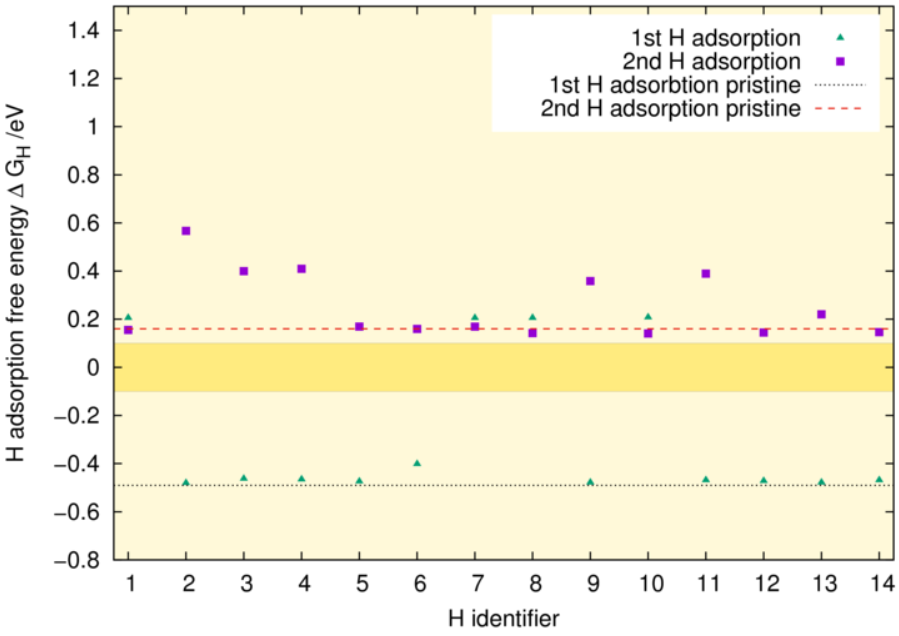


Figure S17: Mo (l2d2)

## 1.2 Dopants on two layers

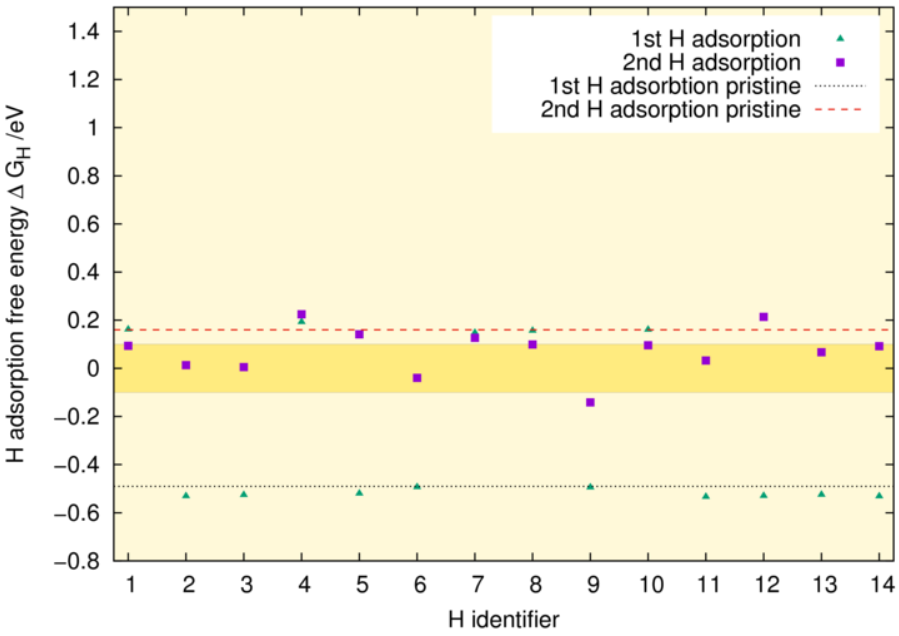


Figure S18: Co (l1l2)

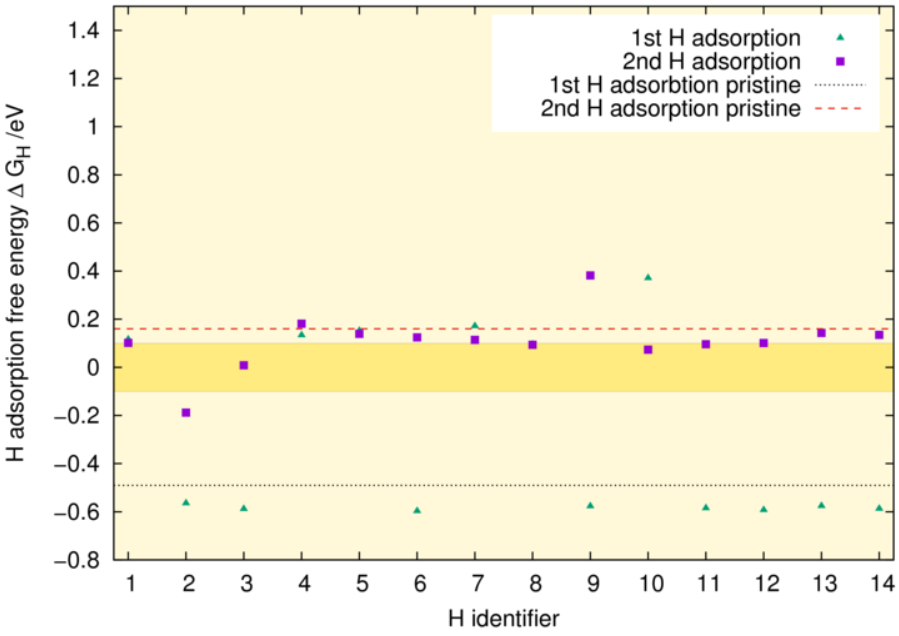


Figure S19: Co (l1l3)

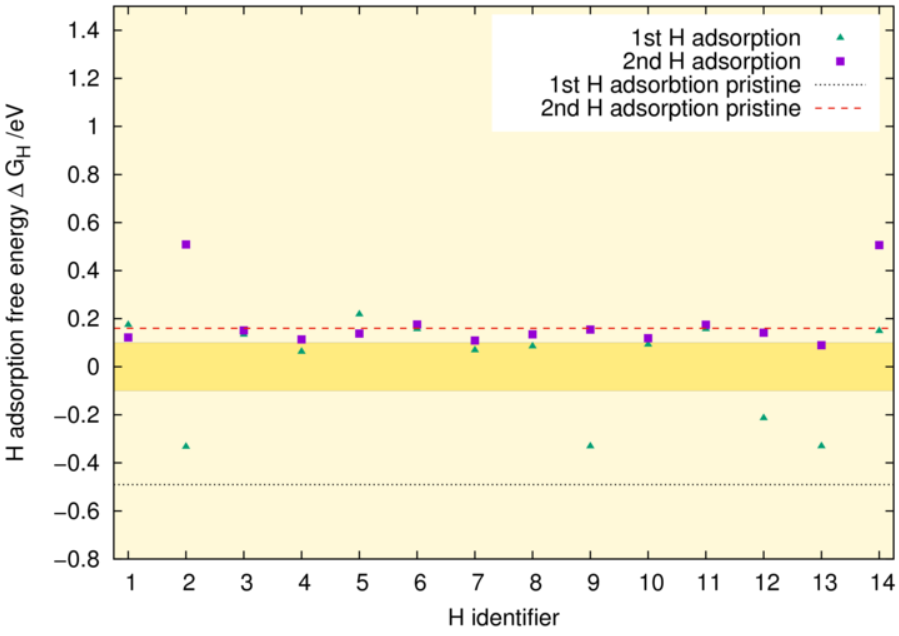


Figure S20: Mg (l2l4)

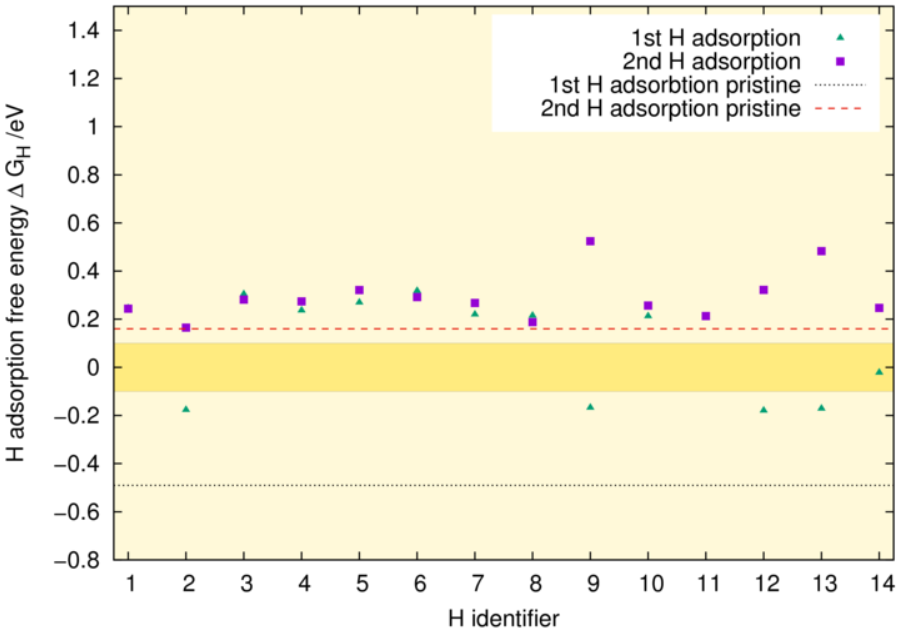


Figure S21: Cu (l1l2)

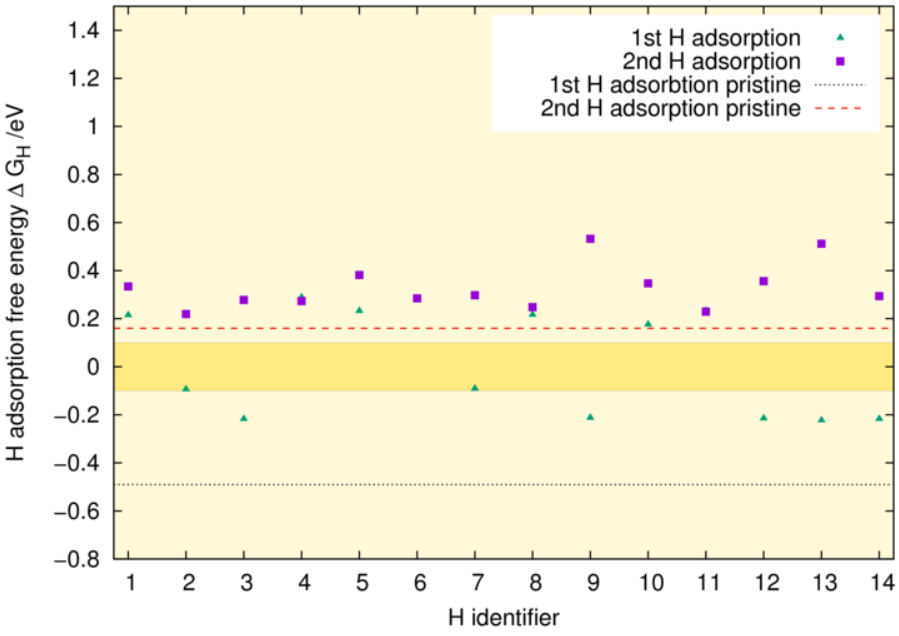


Figure S22: Cu (l1l3)

# 2 H-adsorption energies for $Ni_3P_2$+P termination of $Ni_2P$

Optimised hydrogen adsorption energies for the first (green triangle), second (purple square), and third (red circle) hydrogens at the 14 investigated hydrogen starting positions on top of the $Ni_3P_2$+P terminated $Ni_2P$ slab. The dashed black line indicates the $\Delta G_H$ of the first hydrogen adsorption for the pristine slab, whereas the dashed red line shows the second hydrogen adsorption $\Delta G_H$ value for the pristine slab. As described in the article, the deep yellow band highlights the $\pm 0.1$ eV region around the optimal $\Delta G_H = 0$ value. For example, in Figure S23, the green triangle at H identifier 2 corresponds to the black triangle at Mg (l1d1) in Figure 7 of the main article. Similarly, the purple square at H identifier 12 corresponds to the green square at Mg (l1d1) in the same Figure.

## 2.1 Dopants on a single layer

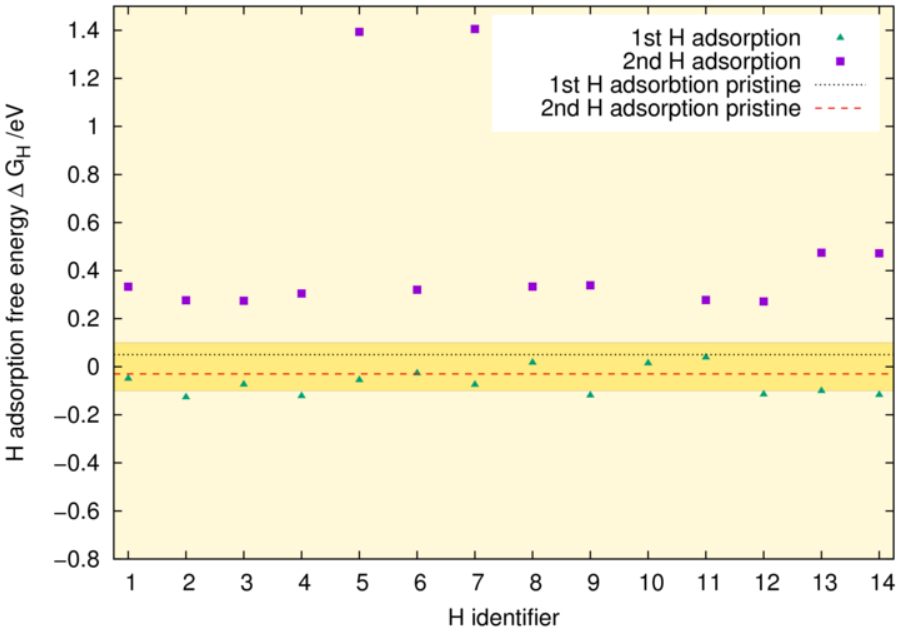


Figure S23: Mg (l1d1)

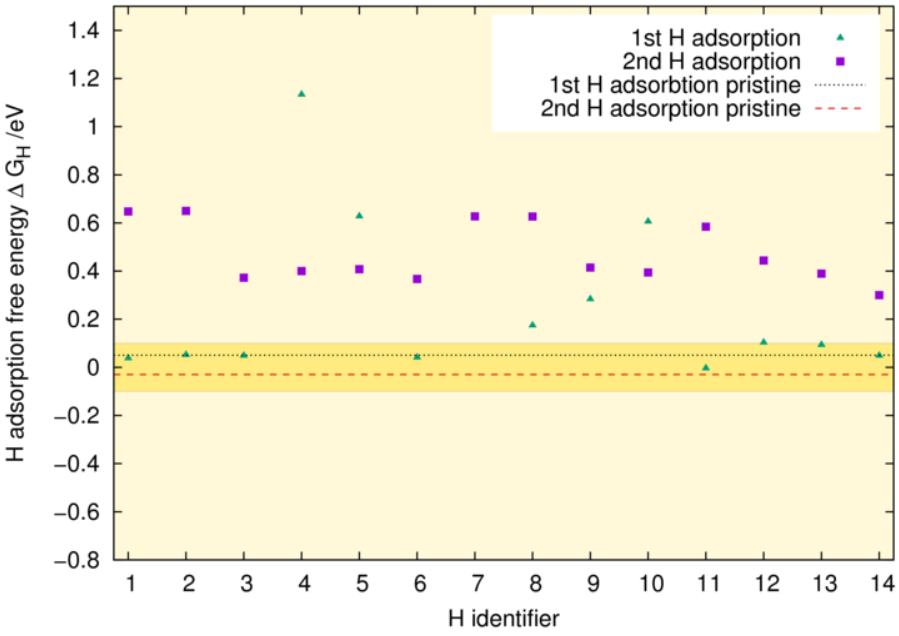


Figure S24: Mg (l1d3)

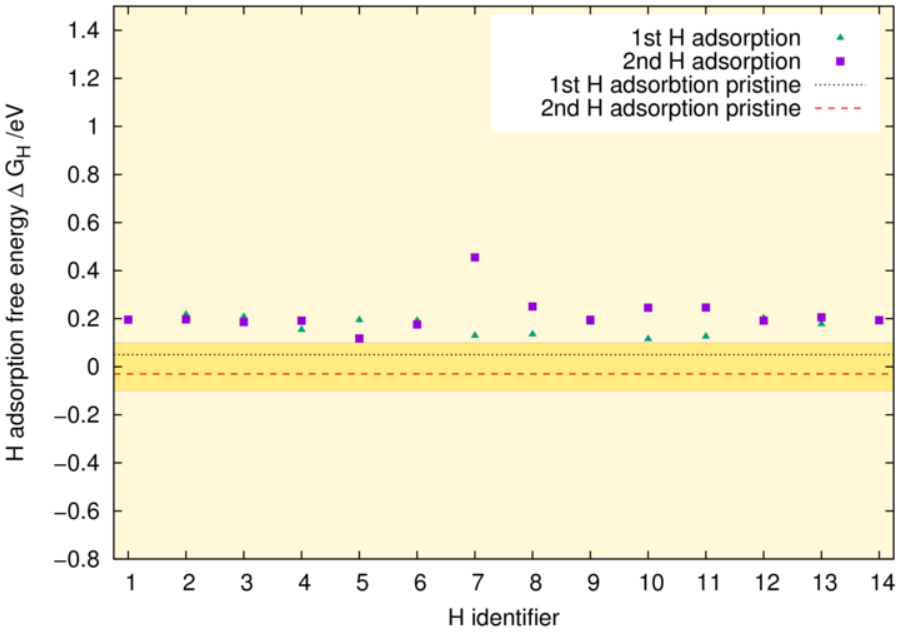


Figure S25: Mg (l2d2)

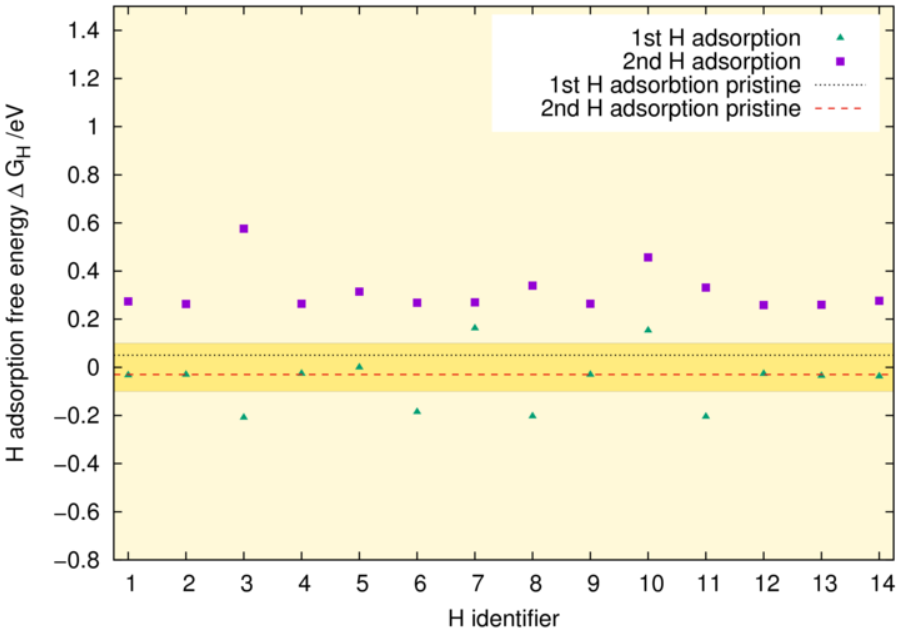


Figure S26: V (l1d1)

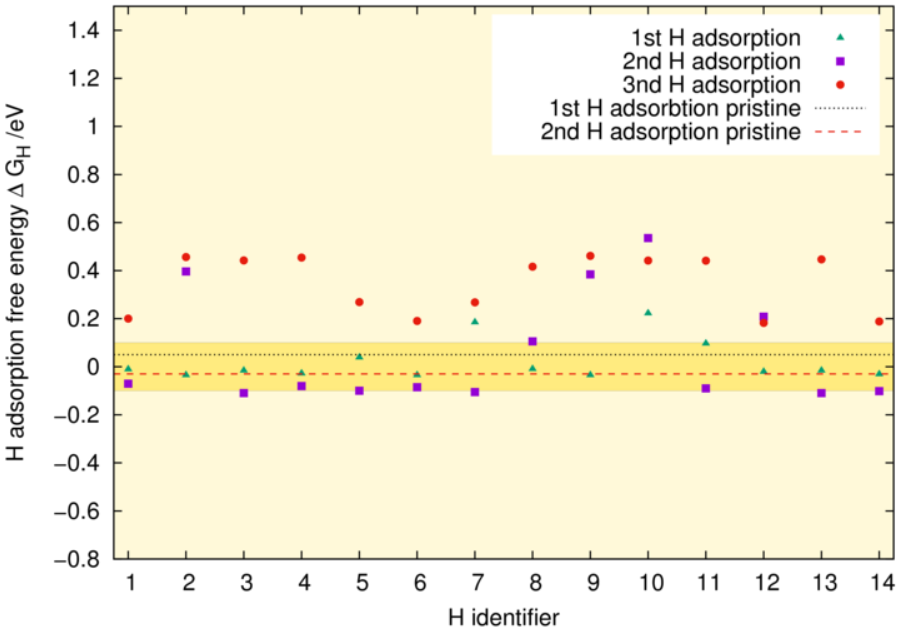


Figure S27: V (l2d1)

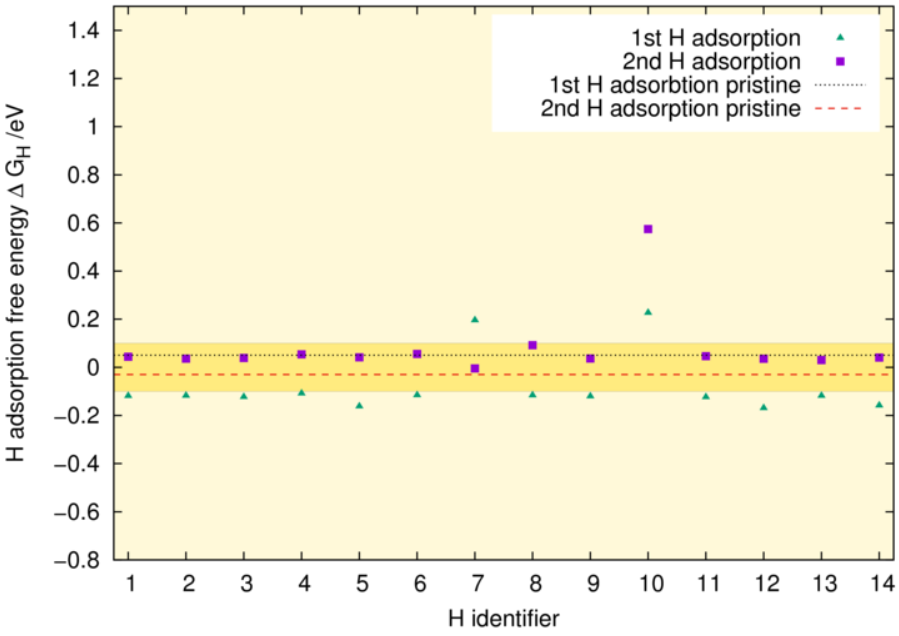


Figure S28: V (l2d2)

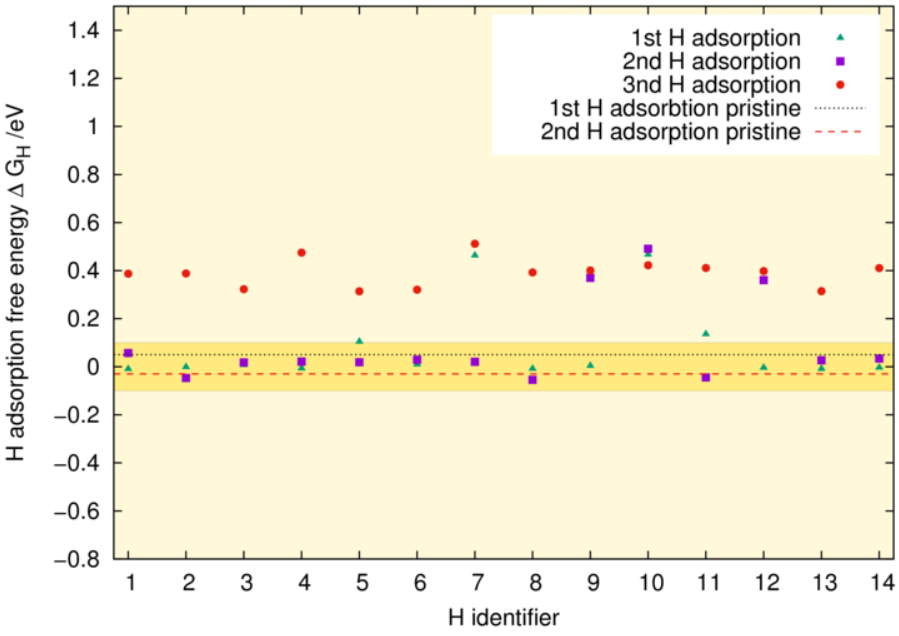


Figure S29: V (l4d1)

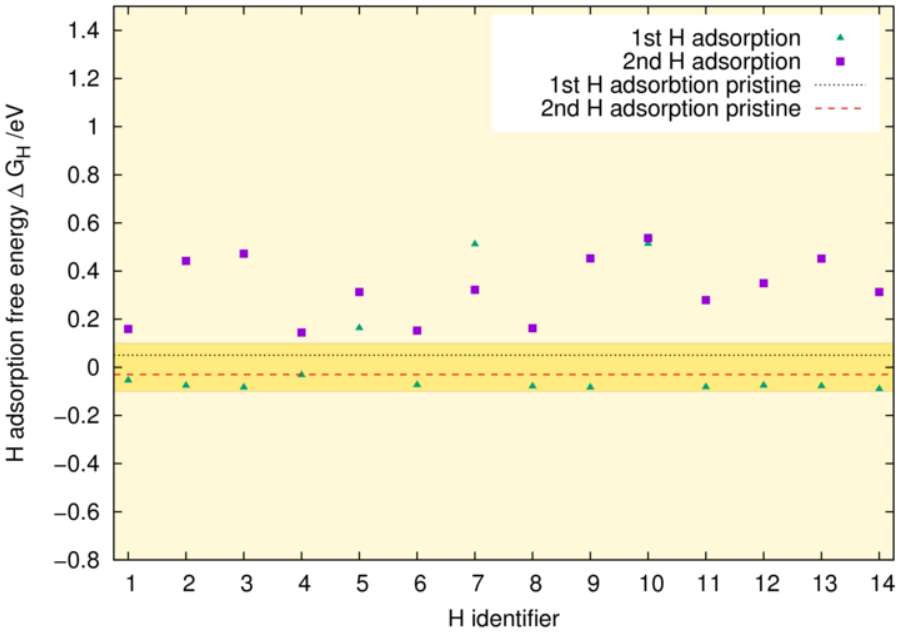


Figure S30: Fe (l1d1)

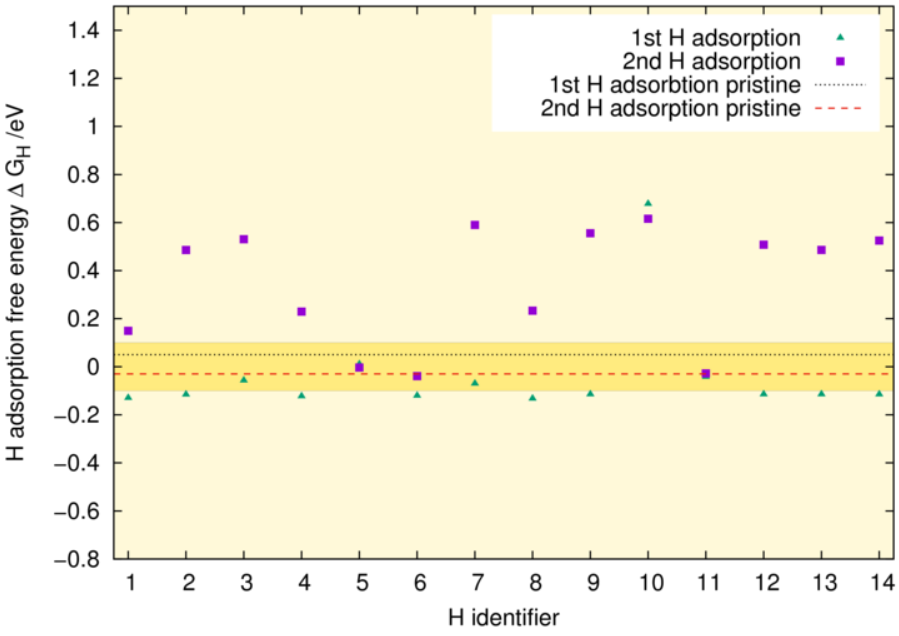


Figure S31: Fe (l1d2)

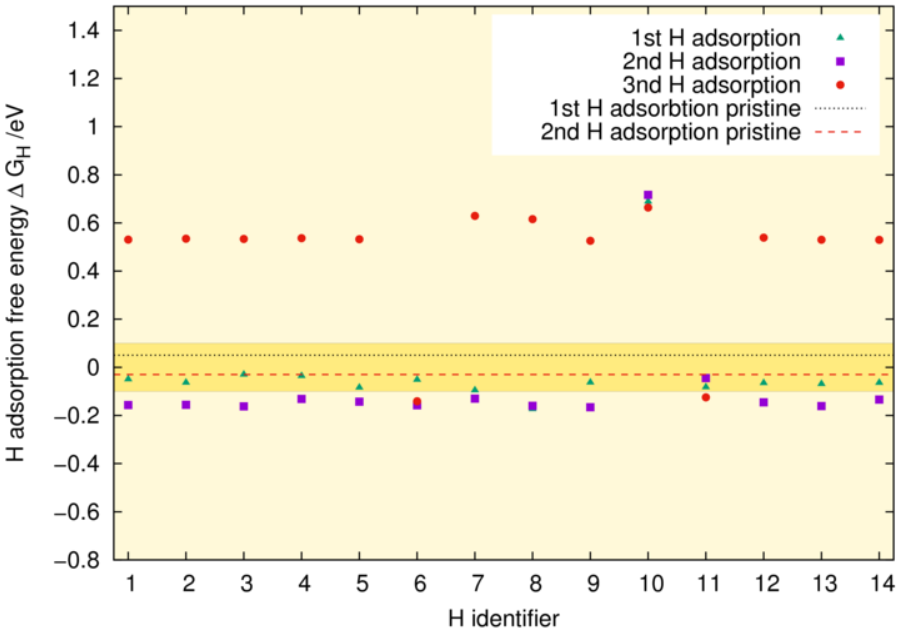


Figure S32: Fe (l1d3)

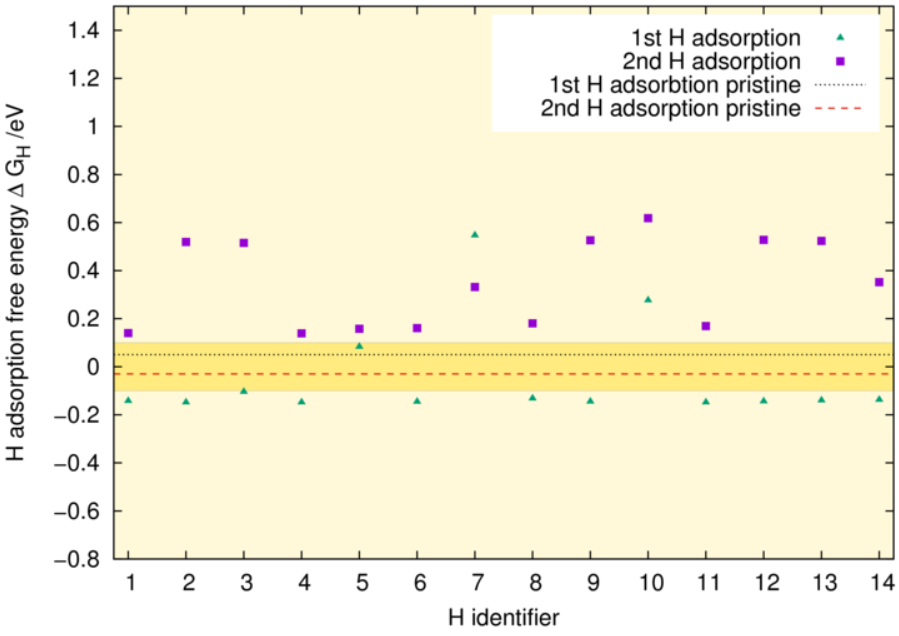


Figure S33: Fe (l3d2)

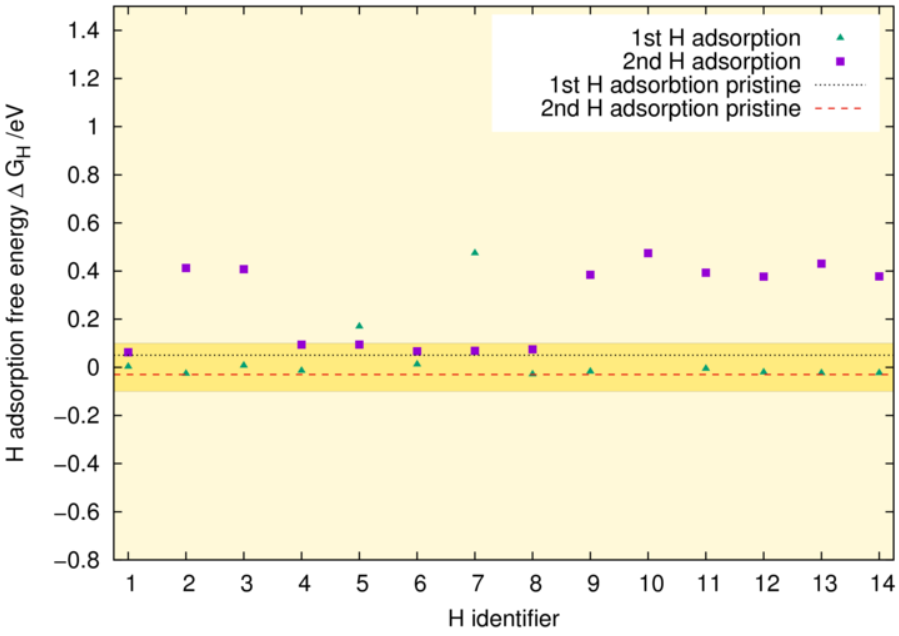


Figure S34: Co (l1d1)

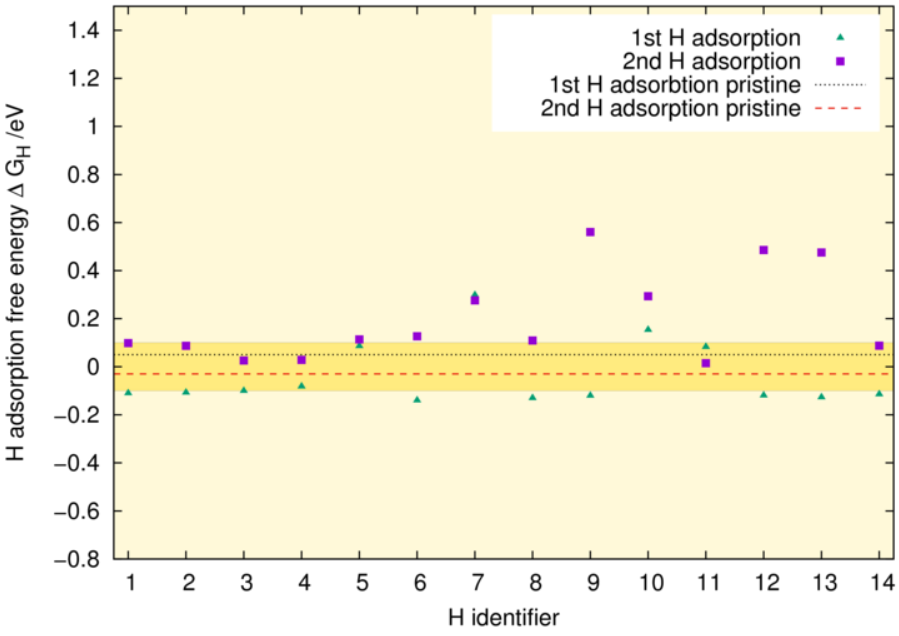


Figure S35: Co (l2d2)

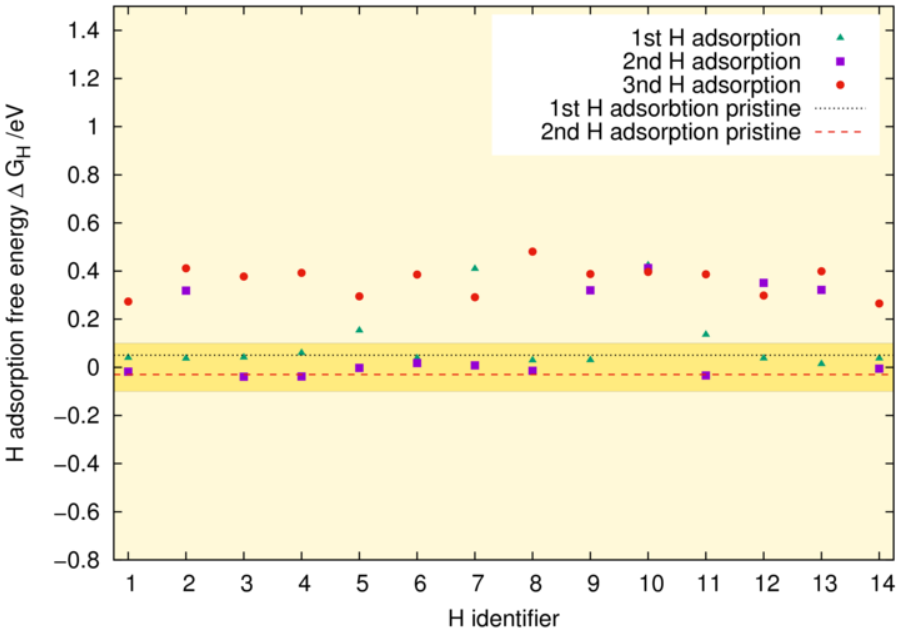


Figure S36: Co (l3d1)

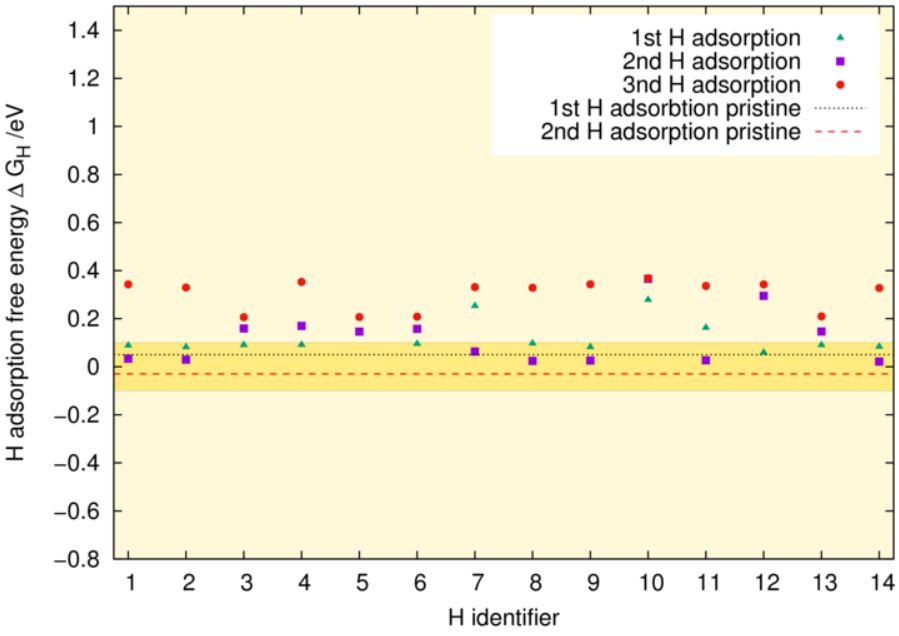


Figure S37: Cu (l2d1)

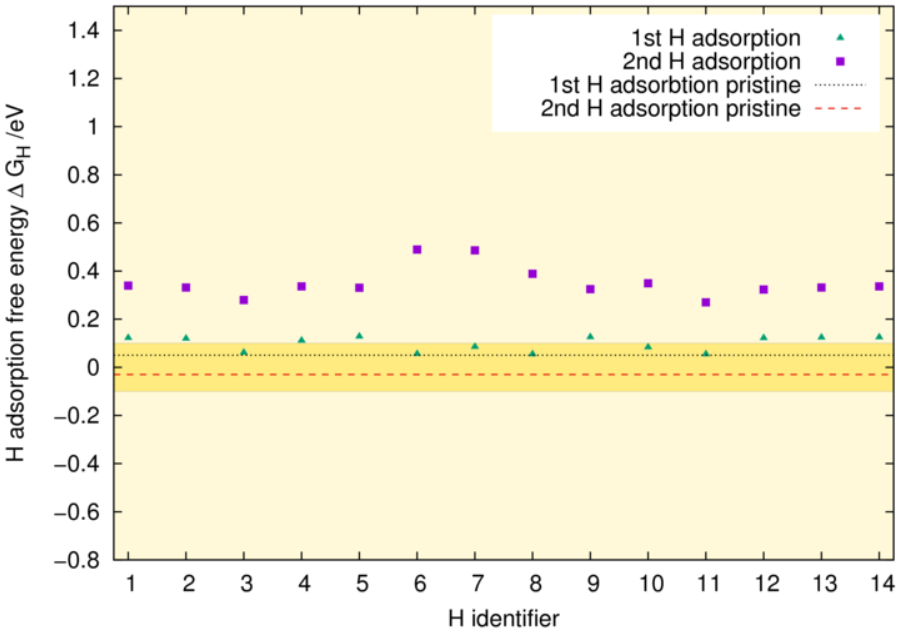


Figure S38: Mo (l1d1)

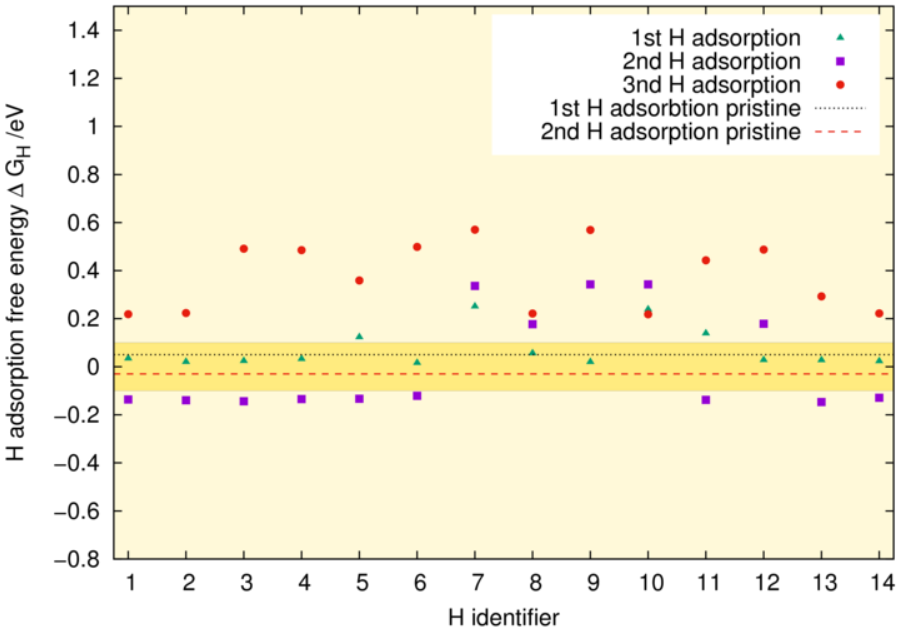


Figure S39: Mo (l2d1)

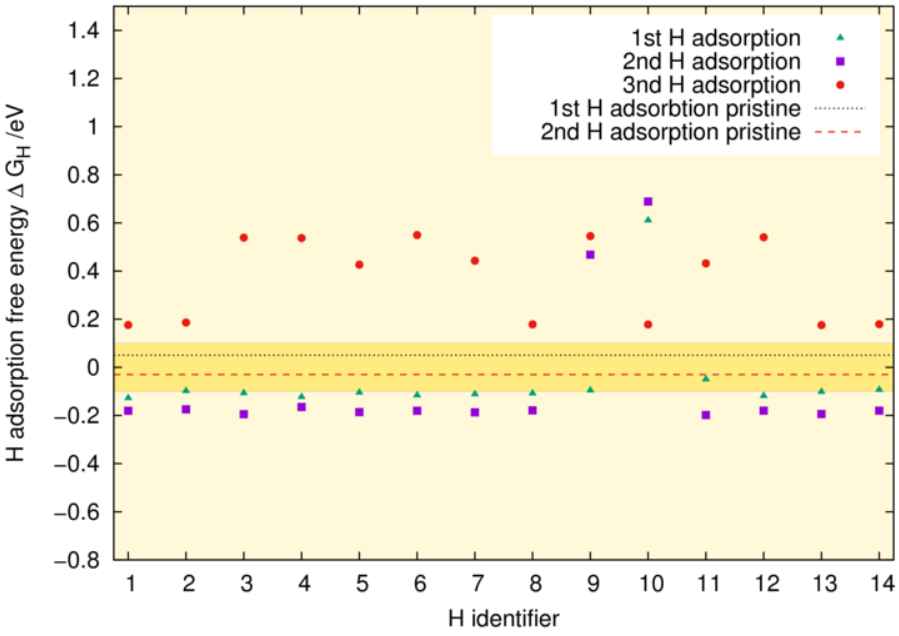


Figure S40: Mo (l2d3)

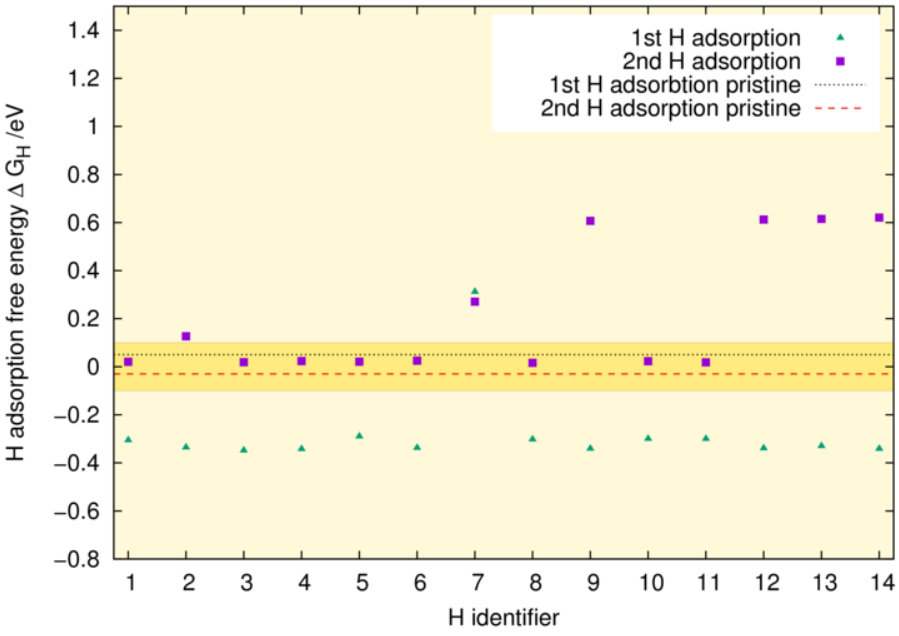


Figure S41: Mo (l3d3)

## 2.2 Dopants on two layers

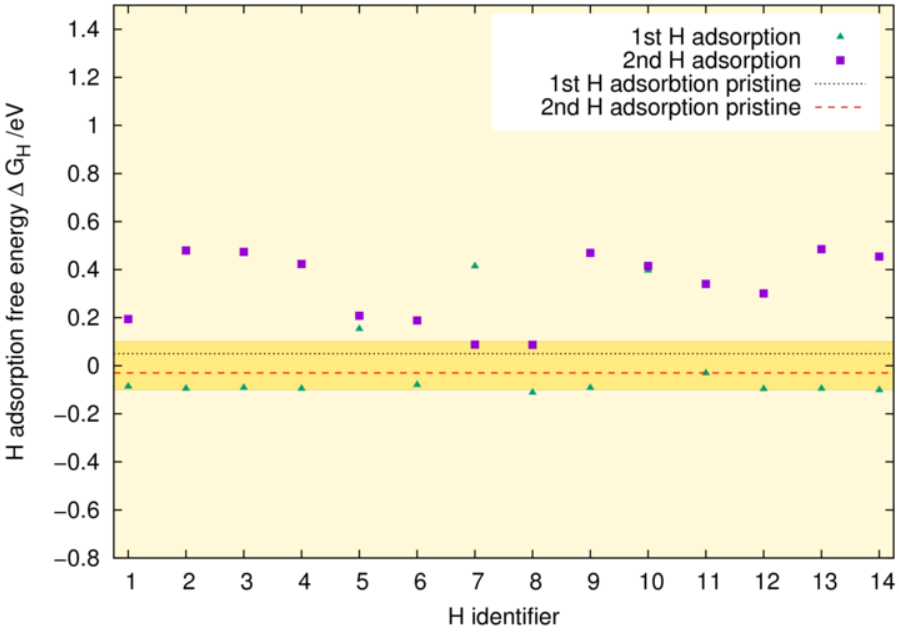


Figure S42: Co (l1l2)